COMPENSATION TEMPERATURE OF A MIXED ISING FERRIMAGNETIC MODEL IN THE PRESENCE OF EXTERNAL MAGNETIC FIELDS.

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ABSTRACT

The behavior of the compensation temperature of a mixed Ising ferrimagnetic system on a square lattice in which the two interpenetrating square sublattices have spins σ $(\pm 1/2)$ and spins S $(\pm 1, 0)$ has been studied with Monte Carlo methods. Our model includes nearest and next-nearest neighbor interactions, a crystal field and an external magnetic field. This model is relevant for understanding bimetallic molecular ferrimagnetic materials. We found that there is a narrow range of parameters of the Hamiltonian for which the model has compensation temperatures and that the compensation point exists only for small values of the external field.

INTRODUCTION

Ferrimagnetic ordering plays a crucial role in stable crystaline room-temperature magnets, that are currently being synthesized by several experimental groups in search for materials with technological applications [1]. In a ferrimagnet the different temperature dependence of the sublattices magnetizations raises the possibility of the appearance of compensation temperatures: temperatures below the critical point, where the total magnetization is zero [2]. The temperature dependence of the coercivity at the compensation point has important applications in the field of thermomagnetic recording [3].

Mixed Ising systems are good models to study ferrimagnetic ordering [4]. Recent results show that these models can have compensation points when their Hamiltonian includes second neighbor interactions [5]. These studies have been performed in zero magnetic field. In this work we study the effect of a constant external magnetic field on the behavior of the compensation temperature, T_{comp}.

THE MIXED ISING MODEL

Our model consists of two interpenetrating square sublattices. One sublattice has spins σ that can take two values $\pm 1/2$, the other sublattice has spins S that can take three values, $\pm 1, 0$. Each S spin has only σ spins as nearest neighbors and vice versa.

The Hamiltonian of the model is given by,

$$H = -J_1 \sum_{\langle nn \rangle} \sigma_i S_j - J_2 \sum_{\langle nnn \rangle} \sigma_i \sigma_k - J_3 \sum_{\langle nnn \rangle} S_j S_l + D \sum_j S_j^2 - h \left(\sum_i \sigma_i + \sum_j S_j \right) \quad (1)$$

where the J's are exchange interaction parameters, D is the crystal field, and h is the external field, all in energy units. We choose $J_1{=}{-1}$ such that the coupling between nearest neighbors is antiferromagnetic.

Previous results with Monte Carlo and Transfer Matrix techniques have shown that the $J_1{-}D$ model (J_2, J_3 and h are all zero) does not have a compensation temperature [6]. These previous studies showed that a compensation temperature is induced by the presence of the next-nearest neighbor (nnn) ferromagnetic interaction, J_2, between the $\pm 1/2$ spins. The minimum strength of the $J_2 > 0$ interaction for a compensation point to appear depends on the other parameters of the Hamiltonian [5]. In this work we study the effect of the external field and the J_3 parameter on the compensation temperature.

MONTE CARLO CALCULATIONS

We use standard importance sampling techniques [7] to simulate the model described by Eq. (1) on $L{\times}L$ square lattices with periodic boundary conditions and L=40. Data were generated with $5{\times}10^4$ Monte Carlo steps per site after discarding the first $5{\times}10^3$ steps. The error bars were taken from the standard deviation of blocks of 500 sites. We define $\beta{=}1/k_{\mathrm{B}}T$ and take Boltzmann's constant $k_{\mathrm{B}}{=}1$. Our program calculates the internal energy per site, specific heat, the sublattice magnetizations per site, M_1 and M_2 defined as,

$$M_1 = \frac{2}{L^2}\langle \sum_j S_j \rangle \quad , \quad M_2 = \frac{2}{L^2}\langle \sum_i \sigma_i \rangle \tag{2}$$

and the total magnetization per spin, $M{=}\frac{1}{2}(M_1 + M_2)$. The averages are taken over all the configurations, the sums over j are over all the sites with S spins and the sums over i are over all the sites with σ spins. Each sum has $L^2/2$ terms.

The compensation point, T_{comp}, is defined as the point where the two sublattice magnetizations cancel each other such that the total magnetization is zero, i.e.,

$$|M_1(T_{\mathrm{comp}})| = |M_2(T_{\mathrm{comp}})| \tag{3}$$

and

$$sign[M_1(T_{\mathrm{comp}})] = -sign[M_2(T_{\mathrm{comp}})] \tag{4}$$

with $T_{\mathrm{comp}}{<}T_{\mathrm{c}}$. Note that at the compensation temperature the sublattice magnetizations are not zero, whereas at the critical temperature, T_{c}, the total magnetization is zero and both sublattice magnetizations are also zero.

RESULTS

Previous studies on the $J_1{-}J_2{-}D$ model showed that, for a fixed value of the parameters J_1 and D, there is a minimum value of J_2 for which the model has a compensation point. However, once this minimum value is reached, the compensation temperature remains almost independent of J_2 [5]. In this study we show that for a fixed value of J_1, D, and J_2, the compensation temperature can be changed by including the J_3 interaction (between the S spins, nnn in the lattice). The effect of the ferromagnetic J_3 parameter is to increase the value of the compensation temperature, such that as J_3 increases the compensation temperature approaches the critical temperature and eventually disappears. In Fig. 1 we show the absolute values of the sublattice magnetizations for a $J_1{-}J_2{-}D$ model (J_3=0, h=0) and for a $J_1{-}J_2{-}J_3{-}D$ model (h=0). Notice that the main effect of the J_3 parameter is to keep the S sublattice ordered at higher temperatures, such that the crossing point between both sublattices [the one that satisfies Eq. (3) and Eq. (4)] occurs at higher temperatures. As J_3 becomes larger, the compensation temperature increases toward the critical point. When

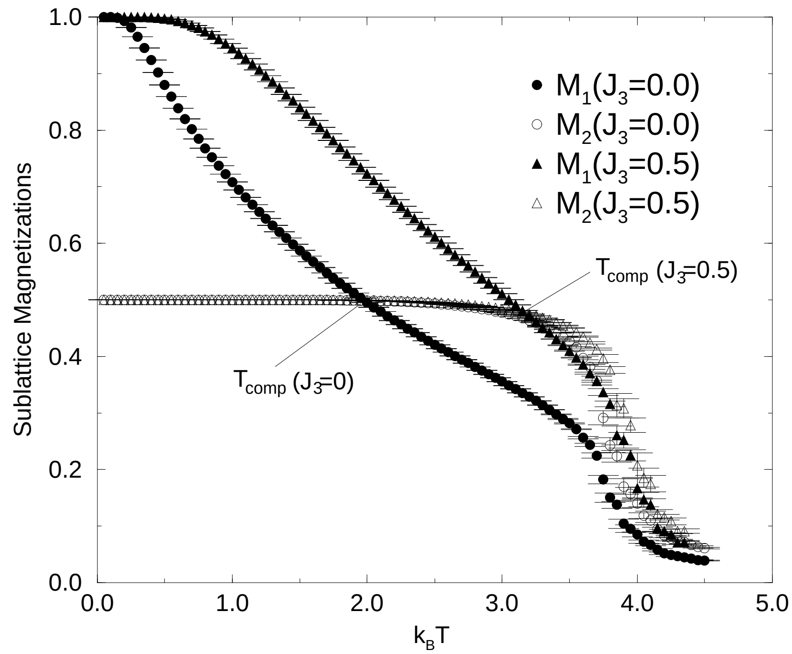

Figure 1: Dependence of the absolute values of the sublattice magnetizations with the temperature for J_3=0 (circles) and J_3=0.5 (triangles). Here J_2=6, D=1 and h=0.

both temperatures become equal we can not talk about a compensation point anymore and we only have a critical temperature.

When an external field h is added, the compensation temperature increases with the field until it disappears, i.e. becomes equal to the critical temperature, for a strong enough value of h, as shown in Fig. 2, where we plot the total magnetization vs. the temperature for several values of h. The effect of the external field on the compensation temperature is similar to that due to J_3. Notice that when h is present the system has a discontinuity in the magnetization that may signal a first order phase transition. This discontinuity seems to be due almost entirely to a discontinuity in the magnetization of the S sublattice as shown in Fig. 3.

In Fig. 4 we show the value of the compensation temperature vs. h for different values of J_3. It is interesting to note that for J_3 fixed the compensation temperature increases almost linearly with the field until it vanishes. Also the compensation temperature increases almost linearly with J_3 for a fixed value of h. As J_3 increases the compensation point only exists for a very weak or zero external field.

CONCLUSIONS

There is a strong dependence of the compensation temperature on the parameters in the Hamiltonian, and only a narrow range of parameters for which a compensation point can exist. The next-nearest neighbor interaction between the S spins and the external magnetic field tend to increase the compensation temperature until it coincides with the critical point, then we no longer have a compensation point. Since the compensation temperature

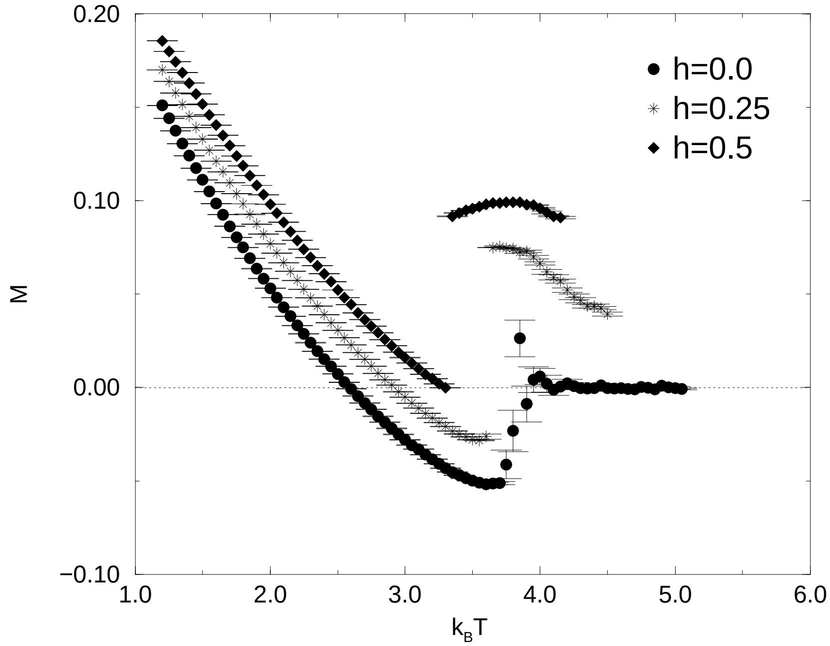

Figure 2: Total magnetizations vs. temperature for different values of h. Here J_3=0.25, J_2=6 and D=1.

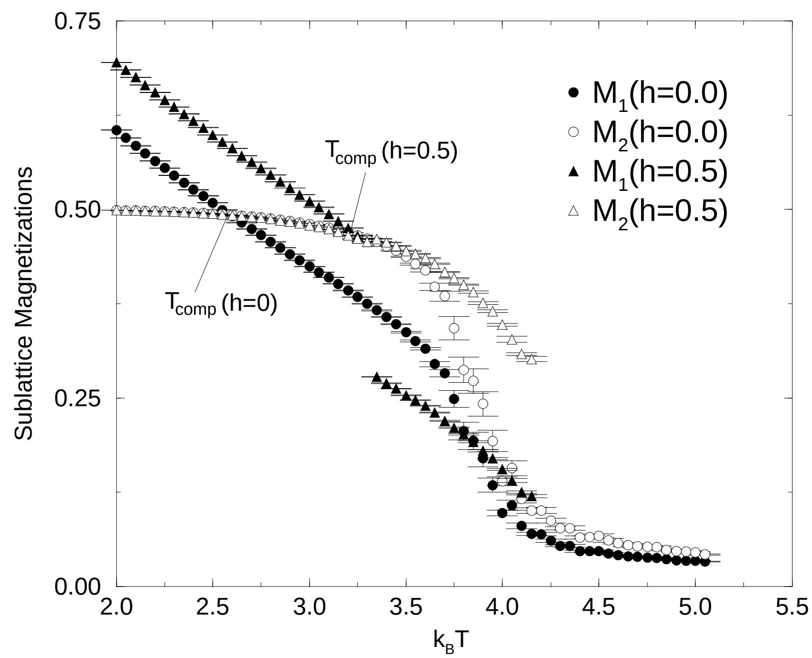

Figure 3: Dependence of the absolute values of the sublattice magnetizations with the temperature for h=0 (circles) and h=0.5 (triangles). Here J_3=0.25, J_2=6 and D=1.

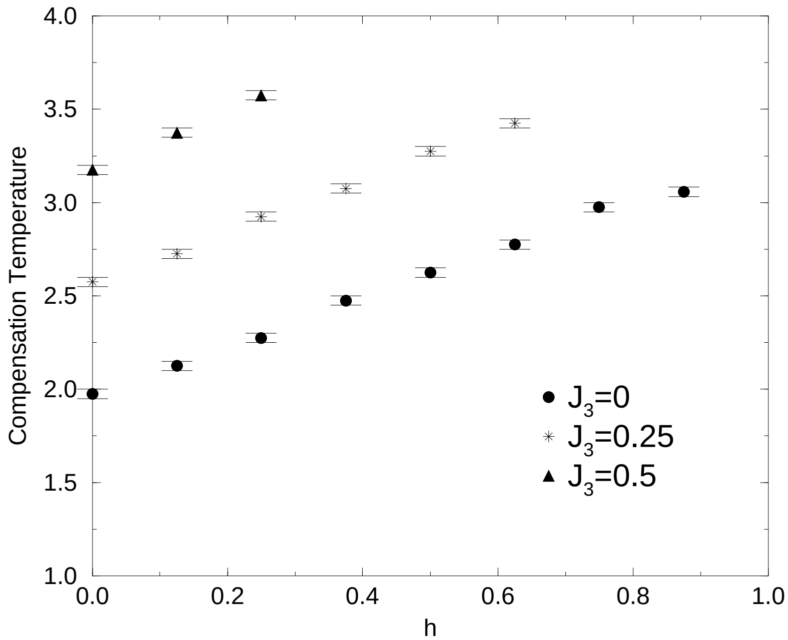

Figure 4: Dependence of the compensation temperature with the external field for different values of J_3. The last point in each curve was calculated at the highest value of h for which there is a compensation point for that particular value of J_3. Here J_2=6 and D=1.

is important in several technological applications, such as thermomagnetic recording, it is important to take into account that the external magnetic fields modify the value of the compensation temperature to higher values and that for strong fields there is no compensation temperature. Also, the presence of magnetic fields seems to induce a discontinuity in the magnetization of the S sublattice.

CONCLUSIONS

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